Ab initio shell-model calculation for ^{18}O in a restricted no-core model space

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We perform an *ab initio* shell-model calculation for ^{18}O in a restricted no-core model space, microscopically deriving a two-body effective interaction and introducing a minimal refinement of one-body energies in the *spsd* or *spsdpf* model space. Low-lying energy levels, except for the experimental 0_2^+ and 2_3^+ states, are better described in the *spsdpf* space than in the *spsd* space. The structure of low-lying energy levels is discussed with an emphasis on many-particle many-hole states beyond the four-particle two-hole configuration.

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The nuclear shell model is a successful method to describe the structure of the nucleus [1, 2]. Recently, the understanding of the nuclear shell structure has been increased by elucidating complicated properties, especially the tensor force, of underlying nuclear interaction [3]. On the other hand, as the numerical calculation becomes larger and more microscopic, the meaning of the word "shell" has become vague. One of the *ab initio* methods to describe nuclei starting with the bare nucleon-nucleon (NN) force in free space is the no-core shell model (NCSM) [4, 5]. In the sense of using harmonic-oscillator (h.o.) Slater-determinant basis states, the NCSM may be regarded as a shell model. However, its basis states span a huge model space, which is taken as large as possible, until the result of the diagonalization converges. Therefore, the meaning of the shell in the NCSM is somewhat different from the usual one in the conventional shell model.

While the formalism of the NCSM for heavier nuclei has been developed, its full application has been limited to nuclei around the mass number $A = 12$ (p-shell nuclei), due to an explosive expansion of the Hamiltonian matrix to be diagonalized. If one explores nuclei heavier than $A = 12$, some approximations or truncations must be employed and the results obtained are no longer exact. However, those results may still contain some important physics. It is well-known that, even in a much more restricted model space, such as the *sd* or *pf* space, the conventional shell-model study with an optimal effective interaction can explain many experimental data [6, 7, 8, 9]. Thus, it is our purpose in this study to bridge the gap between the two approaches.

Recently, some attempts have been proposed along this line. One is a shell-model calculation in the no-core *spsdpf* space combined with a minimal refinement of the one-body energies [10]. This no-core type of shell model has been applied to the neutron-rich carbon isotopes around ^{16}C, and it has been shown that low-lying energy levels are well described. Another is an *ab initio* shell model with a core in which a p-shell effective Hamiltonian for light nuclei is constructed utilizing a NCSM result in a sufficiently large model space [11]. In both methods, no experimental information about the energy levels is used, and a double unitary transformation is performed to microscopically derive the effective interaction. In this Letter, we employ the former method and investigate the structure of ^{18}O.

Since ^{18}O is a typical *sd*-shell nucleus, which has the structure of two neutrons and a core nucleus, there have been many theoretical studies. As for the shell model with a microscopic effective interaction, the work of Kuo and Brown is the pioneering study [12]. They constructed the effective interaction for the *sd* model space and showed that low-lying energy levels are well described. However, even in this early stage, the importance of including a larger space for the intermediate states in determining the effective interaction was pointed out by others [13, 14].

In Ref. [15], a recent *sd* shell-model calculation for ^{18}O using a modern NN interaction with the folded diagram theory has been reported. Although this method seems to be successful in describing low-lying energy levels, intruder states having many-particle many-hole dominant configurations may not be properly reproduced due to the limited *sd* model space. If one wants to describe such many-particle many-hole states explicitly, several major shells must be included in the model space. In this sense, our present work in a *restricted* no-core model space would be preferable for the simultaneous description of the ground and complicated excited states.

Here, we outline the method of deriving the effective interaction in our restricted no-core space. The details are given in Refs. [10, 16]. First we derive the two-body effective interaction from a realistic NN interaction in a large model space P_1, solving the decoupling equation [17] between the model space P_1 and its compliment Q_1. The P_1 space consisting of the two-body states is defined by a boundary number $\rho_1 \leq 2n_1 + l_1 + 2n_2 + l_2$ with the h.o. quantum numbers $\{n_1, l_1\}$ and $\{n_2, l_2\}$ of the two-body states. Note that the full space of the two-body states $P_1 + Q_1$, which is necessary to accurately take into account the strong repulsion effect of the NN force at short

distance reaches about 300 $\hbar\Omega$ in h.o. energy. Therefore, in general, the diagonalization of the original many-nucleon Hamiltonian in such an energy range could not be performed in the foreseeable future. The effective interaction determined in this first step corresponds to a well-behaved interaction that renormalizes the effect of the short-range repulsion.

If one uses this effective interaction for a sufficiently large model space in the diagonalization of the Hamiltonian, this leads to the NCSM. However, this type of approach cannot be applied to heavier nuclei, since the dimension of the matrix becomes huge. Therefore, in order to construct an effective interaction suitable for a no-core type of shell-model calculation in a tractable model space, we again solve the decoupling equation between a smaller model space P_2, such as the *spsd* or *spsdpf* space, and its compliment Q_2 using the two-body effective interaction determined in the first step, where $P_1 = P_2 + Q_2$. Note that the boundary number ρ_1 is taken to be $\rho_1 = 6$ in the present work and, thus, is not so big, although this number should be taken as large as possible in the usual sense of the NCSM. The smaller model space P_2 and its compliment Q_2 are not separated by energy but by state, and, thus, some two-body states in the model space are degenerate with those in its complement. This degeneracy often causes a difficulty in determining the effective interaction. Furthermore, in contrast to the usual NCSM, we solve the decoupling equation by introducing a self-consistent one-body potential for ^{16}O and use it to construct a suitable effective interaction in the small model space for nuclei around ^{16}O. This self-consistent procedure also makes the problem more difficult to solve, if the degeneracy is big. Thus, in this second step of the calculation, the self-consistent potential is introduced only for the small model space P_2. The self-consistent potential is also calculated for the large model space P_1 in the first-step decoupling. Although we decided to take the *small* number $\rho_1 = 6$ to make the degeneracy as small as possible, this artificial truncation is compensated to some extent by introducing a minimal refinement of one-body energies as explained later.

Consequently, our shell-model Hamiltonian is composed of the sum of the one-body kinetic energy (the minimal refinement of one-body energies), the two-body effective interaction for the P_2 space, and the center-of-mass (c.m.) Hamiltonian which is multiplied by a large value $\beta_{\rm c.m.}$ to separate the spurious c.m. motion from the physical states [18].

In this work, we use the CD-Bonn potential [19] as the original NN interaction. In Fig. 1, we present the dependence of the ground-state energy of ^{18}O on the h.o. frequency $\hbar\Omega$. The effect of the minimal refinement has not yet been included in the results. The results for three different model spaces used in the diagonalization are shown: up to the four-particle two-hole (4p2h) configuration in the *spsdpf* space, the 4p2h *spsd*, and the 6p4h

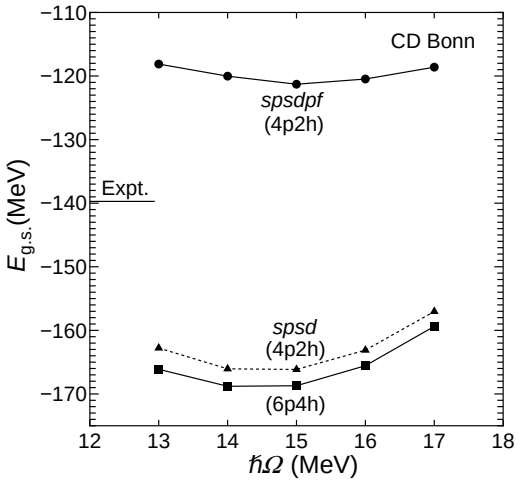

FIG. 1: The $\hbar\Omega$ dependence of the calculated ground-state energies of ^{18}O.

spsd from the unperturbed ground state of ^{16}O. The result at the energy minimum point for the *spsdpf* space shows a less attractive energy by about 20 MeV than the experimental value, while the results for the *spsd* space are much more attractive. It is known that the CD-Bonn potential underbinds nuclei in high-precision calculations for few-nucleon systems. Our result for the *spsdpf* space is consistent with this tendency. As expected, the *spsdpf* result is more favorable than the *spsd* results. In the *spsd* calculations, the overbinding of the energy could be compensated by introducing a repulsive and sizable three-body effective interaction, but such a calculation cannot be easily done. For all three types of calculation, there appear energy minima at around $\hbar\Omega = 15$ MeV. Therefore, we choose this value as the optimal one for all the results in this study.

The ground-state energy for the 4p2h *spsdpf* case at the optimal value of $\hbar\Omega$ is about -120 MeV. We note, however, that this number has an ambiguity due to several effects. In addition to some approximations and truncations in deriving the effective interaction and performing the diagonalization, there is a problem regarding the removal of the spurious c.m. motion. Unlike the usual NCSM approach, our shell-model space is not given by energy but by state. In such a state separation, the influence of the spurious c.m. states on the energy levels of intrinsic states cannot be completely removed by a suitable value of $\beta_{\rm c.m.}$. This problem has recently been examined in NCSM and coupled-cluster calculations by Roth *et al.*, and they have shown that the c.m. effect is non-negligible in restricted and incomplete energy spaces [20]. However, if we look at the relative structure from the ground state, this effect is expected to be small for a sufficiently large value of $\beta_{\rm c.m.}$, as in the study of carbon isotopes [10].

In the calculation of the energy levels of ^{18}O, it is im-

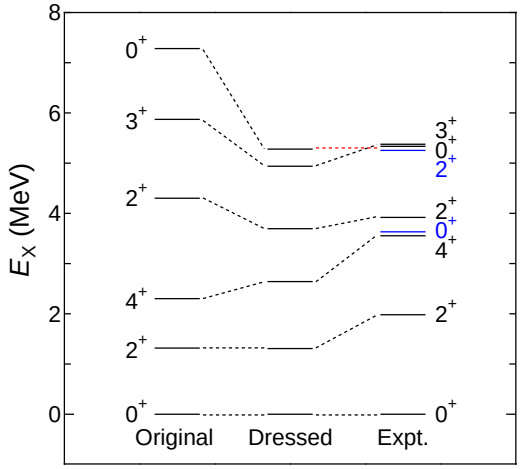

FIG. 2: Low-lying energy levels of the positive-parity states in ^{18}O.

portant to investigate the neutron single-particle energies for the lowest three states in ^{17}O. If the calculated single-particle levels in ^{17}O are not comparable to the experimental values, the calculation for ^{18}O would be questionable. We have found that, in the present shell-model space, the calculated single-particle levels are not so satisfactory. On the other hand, we know that, if we compute the single-particle energies using the CD-Bonn potential within the framework of the unitary-model-operator approach (UMOA), the results are close to the experiments [16]. The UMOA can be regarded as a sort of e^S method or coupled-cluster theory of the Hermitian type [21]. In the UMOA, the calculation of the single-particle energy is feasible in a sufficiently large model space, although it is hard to obtain complicated states. Therefore, in order to include the effect of the correlation energy of the large space into the present restricted one in a simple way, we change the one-body matrix elements of the neutron in the *sd* shell, utilizing single-particle information obtained by the UMOA. This variation is the "minimal refinement".

The magnitude of the minimal refinement is determined so as to reproduce the binding energies of the lowest single-particle $5/2^+$, $1/2^+$, and $3/2^+$ states in ^{17}O obtained within the UMOA, as a consequence of the shell-model diagonalization in the present space. Denoting the one-body energy for a single-particle orbit j of the neutron as $\epsilon^n(j)$, we need these variations for the 4p2h *spsdpf* case to be $\Delta\epsilon^n(0d_{5/2}) = 0.99$, $\Delta\epsilon^n(1s_{1/2}) = -0.42$, and $\Delta\epsilon^n(0d_{3/2}) = -1.04$ MeV. These are added to the original $\epsilon^n(j)$'s, namely, the h.o. kinetic energies. We have checked that the results for the excited state energies above the ground state are hardly changed, even if we introduce similar refinements into the proton orbits of the *sd* shell and the hole orbits for the neutron and the proton.

In Fig. 2, we illustrate calculated low-lying energy spectra of the positive-parity states for the 4p2h *spsdpf* case, together with the experimental levels. The energy levels in the first and second columns, labeled by "Original" and "Dressed", denote the results without and with the minimal refinement, respectively. For the case "Original", the excited levels above $E_X = 3$ MeV lie higher than the corresponding experimental ones, while those below $E_X = 3$ MeV lower than the experiments. By introducing the minimal refinement, the results on the whole become closer to experiment. A similar tendency was seen in the calculation for the neutron-rich carbon isotopes [10].

TABLE I: The excitation energies of low-lying positive-parity states in ^{18}O. The calculated results are for the cases (a) 4p2h *spsd*, (b) 6p4h *spsd*, and (c) 4p2h *spsdpf*. All energies are in MeV.

J^π	(a)	(b)	(c)	Expt.
3^+	3.68	3.84	4.94	5.38
0^+	4.13	4.36	5.28	5.34
2^+				5.25
2^+	3.00	3.09	3.70	3.92
0^+				3.63
4^+	1.48	1.57	2.64	3.55
2^+	0.67	0.74	1.31	1.98

To demonstrate the advantage of the calculation in the *spsdpf* space over the *spsd*, as in Fig. 1, the results of the low-lying energy levels for the three spaces in the "Dressed" case are given in Table I. Note that the magnitudes of the minimal refinement of the one-body energies depend on the model-space size employed. The magnitudes for the 4p2h *spsdpf* have been given before; those for the 4p2h *spsd* are $\Delta\epsilon^n(0d_{5/2}) = 2.12$, $\Delta\epsilon^n(1s_{1/2}) = -3.14$, and $\Delta\epsilon^n(0d_{3/2}) = -1.81$ MeV, and for the 6p4h *spsd*, $\Delta\epsilon^n(0d_{5/2}) = 2.42$, $\Delta\epsilon^n(1s_{1/2}) = -2.59$, and $\Delta\epsilon^n(0d_{3/2}) = -1.30$ MeV. These values are determined in each restricted model space so as to reproduce the UMOA results. The energy spacings for the 4p2h *spsd* case are rather compressed compared to the experimental data. The inclusion of the $6p4h$ configuration does not cause any significant change in the relative spacings. The results for the 0_2^+ state for the *spsd* cases are fairly close to the experimental 0_2^+ rather than the experimental 0_3^+. However, by including the pf shell, the calculated 0_2^+ state becomes close to the experimental 0_3^+, and the energy spacings are expanded. Then the results become, on the whole, close to the experimental values. This suggests the risk of using the experimental single-particle energies in the conventional shell model, leading to an accidental reproduction of energy levels of the wrong structure [22].

As shown before, the minimal refinements for the *spsd* cases are considerably larger than the *spsdpf* ones. This means that the minimal refinements in the *spsd* cases are not so realistic. In general, the effect of the many-

TABLE II: The excitation energies $E_{\rm x}$ in MeV and the probabilities of the 4p2h configuration $P_{\rm 4p2h}$ for the lowest 4p2h-dominated 0^+ state in ^{18}O, for the configurations up to 4p2h, 6p4h, and 8p6h in the *spsd* space.

Configuration (*spsd*)	4p2h	6p4h	8p6h
$E_{\rm x}$	41.75	31.50	30.29
$P_{\rm 4p2h}$	0.996	0.855	0.816

body effective interaction becomes bigger as the size of the model space becomes smaller. Therefore, in the *spsd* space, the change of only the one-body energy may be too simple a treatment. In such a small model space, we should change not only the one-body energy but also the two-or-more-body matrix element.

Interestingly, in the *spsdpf* case, the result of the 0^+_2 state appears at near the experimental 0^+_3, and there is no calculated 0^+ state near the experimental 0^+_2. Furthermore, we cannot find a 2^+ state near the experimental 2^+_3. These experimental 0^+_2 and 2^+_3 levels have been treated as (deformed) 4p2h states in shell-model calculations [22], while these states have been considered to be well-developed ^{14}C+α cluster states in Refs. [23, 24]. In our calculation, the 4p2h configurations are included. Nevertheless, there occurs no indication that our 4p2h states come down to the low-lying energy region.

There may be some reasons for the disappearance. One is the simple treatment of the minimal refinement, even in the *spsdpf* space. Another is the effect of higher configurations, such as the 6p4h, on the 4p2h dominant state. To investigate this effect, we have calculated the lowest $4p2h$-dominated state in the *spsd* case. In Table II, we tabulate the excitation energies and the probabilities of the 4p2h configuration for the lowest 0^+ state dominated by the 4p2h configuration, for the configurations up to 4p2h, 6p4h, and 8p6h in the *spsd* space. The probabilities of the 4p2h configuration contain the contributions from all the 4p2h states in each space. The calculated 4p2h state is the fourth 0^+ state in the *spsd* case. The third 0^+, which is dominantly composed of the $(0d_{3/2})^2$ configuration of the neutron, lies at about 16 MeV in excitation energy for the three cases. Although the excitation energies in Table II are far from the experimental 0^+_2, a considerable contribution of about -10 MeV from the 6p4h configuration is brought to the excitation energy, while that from the 8p6h configuration is rather small. This indicates the importance of also including the 6p4h in larger spaces, even if the $4p2h$ is the dominant configuration, when (spherical) h.o. wave functions are used as the basis states. Such a calculation is a challenging problem to reveal the real structure of the experimental 0^+_2 and 2^+_3 states.

In conclusion, low-lying states in ^{18}O are well described by our *ab initio* shell-model calculation with minimal refinement in the no-core *spsdpf* space. However, a larger model space is necessary to properly describe the experimental 0^+_2 and 2^+_3 states.

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